MULTIALIQUOT CELL APPROACH FOR THE SDPD OF HIGH SYMMETRY COMPOUNDS

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Recently mentioned [1] inconsistency of figures of merit [2,3] when indexing high symmetry lattices turned to a conclusion the smaller cells of lower symmetry can be applied as building units when solving a structure by direct space methods. The approach is expected to decrease time necessary for simulated annealing of a structure solution and may appear particularly useful for large organic structures. The poster illustrates the approach based of example compounds with a reatively small pyrochlore structure. The indexing program suggests several possible solutions and the correct solution of highest symmetry among them. The repetition of the same lattice described by different cells should be considered as an indication of the correct indexing solution. The extension to indexing algorithms, eliminating lower symmetry cells for the same lattice described by high-symmetry cell, and the corrected figures of merit taking into account the number of equal proposal cells might be drawn as follows:

$$M_{sm} = \sum M(20)_i$$
$$F_{sm} = \sum F(20)_i$$

where $M(20)_i$ and $F(20)_i$ are M(20) and F(20) for the aliquot cells

Then, one may start to search for the structural model applying a cell of lower/volume symmetry providing it may represent a building unit for the larger cell of higher symmetry or may asssist to find a sublattice. In an example pyrochlore compound, indexing program points to an unit of a' = a/4 size and V' = V/64, representing an A_6 or a B_6 tetrahedra.

[1] O.A. Smirnova, in Abstracts, Denver X-ray conference 2009, Colorado Springs 2009, USA.
[2] De Wolff, P.M., J. APPL. CRYST. 5, 108-113 (1968).
[3] Smith, G. S. & Snyder, R. L., J. APPL. CRYST. 12, 60-65 (1979).